Polynomial scheme for time evolution of open and closed quantum systems

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Based on the generating function of Laguerre polynomials, we propose a Laguerre polynomial expansion scheme in the calculation of the evolution of the time-dependent Schrödinger equation. Theoretical analysis and numerical tests show that the method is equally as good as the Chebyshev polynomial expansion method in efficiency and accuracy, with the additional merits that no scaling to the Hamiltonian is needed and it has wider suitability.

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I. INTRODUCTION

Studies of open quantum systems have a long history [1]. There has been renewed interest in recent years due to the development of the concept and possible realization of quantum communication and quantum computation [2,3]. A key concept in the study of open quantum systems is the decoherence of a quantum system interacting with environments, which plays a very important rule in almost all phenomena in the quantum devices used in quantum computation and quantum communication [4–6]. It has been shown that the states of an open quantum system will finally relax into a set of "pointer states" in the Hilbert space [5] by decoherence, i.e., for a quantum system prepared in a linear superposition of its eigenstates, interaction of the system with its environment results in a decay from the system's initial pure state $\rho_s(t=0)=|\psi_0\rangle\langle\psi_0|$ to a mixed state $\rho_s(t>0)=\Sigma_i p_i\rho_i$, $\Sigma_i p_i=1$. To be specific, an arbitrary initial state of the system plus the environment may be written as

$$|\psi(t=0)\rangle=\left(\sum_n C_n|n\rangle\right)\otimes|\psi_e\rangle, \tag{1}$$

where the set $|n\rangle$ stands for the eigenstates of the system and $|\psi_e\rangle$ is the initial state of the environment. This state at time t larger than the decoherence time τ_d evolved to a mixed state, which may be expanded as

$$|\psi(t)\rangle=\sum_m C_m(t)(|m\rangle\otimes|e_m\rangle). \tag{2}$$

Here, the set of states $|m\rangle$ are the so-called pointer states of the system [7–9], and $|e_m\rangle$ are the corresponding states of the environment that are entangled with $|m\rangle$ [10]. A convenient way to represent the system interacting with the environment is the reduced density matrix, defined as

$$\rho_s=\mathrm{Tr}_e[|\psi(t)\rangle\langle\psi(t)|],$$

where Tr_e means tracing over the environment degrees of freedom. The evolution from (1) to (2) may be rewritten as

$$\rho_s(0)\Rightarrow\rho_s(t)=\sum_m|C_m(t)|^2|m\rangle\langle m|. \tag{3}$$

When the time $t\gg\tau_d$, the nondiagonal elements of the reduced density matrix $\rho_s(t)$ vanish and the diagonal elements achieve their equilibrium values. This effect of decoherence is typical for all known quantum systems, and induces an increase of the system's entropy and the damping of quantum oscillations with time [11,12].

A theoretical description of the evolution of the system from $\psi(0)$ to $\psi(t)$ driven externally by the environment is generally a very difficult problem. The case that the environment is described by boson fields has been extensively studied in the context of the master equation approach, with both Markovian [7] and non-Markovian [13] approximations. Although the master equation scheme can be used for a large number of environments of different types (phonon, photons, etc.) [12], the master equation description is not universally valid for all the models of environment and is fragile in some systems [14].

Generally, if the Hamiltonian of the compound system is known, the direct way to solve the decoherence problem is to follow the evolution of the compound system over a substantial period of time. By setting $\hbar=1$, the time-dependent Schrödinger equation is

$$i\frac{\partial\psi(t)}{\partial t}=\hat{H}\psi(t). \tag{4}$$

Here $\hat{H}$ is the total Hamiltonian of the system plus the environment. Equation (4) can be decomposed into a set of first-order ordinary differential equations with the initial condition $\psi(0)$, and the total number of equations is the dimension of the Hilbert space of the whole system, which is usually very large. In principle, the set of equations can be solved by convenient methods of ordinary differential equations such as the predictor-corrector or Runge-Kutta method. However, direct solution of the equations will cost too much computer resource due to the large number of equations involved. Another scheme for propagating Eq. (4) is to expand the evolution operator $U(t)=\exp(-i\hat{H}\Delta t)$ in a Taylor series, where Δt is the time step:

$$\exp(-i\hat{H}\Delta t)=1-i\hat{H}\Delta t+\cdots. \tag{5}$$

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It has been stated in Ref. [15] that a numerical scheme based on this expansion is not stable, because it does not conserve the time reversal symmetry of the Schrödinger equation. Variations of the Taylor series have been proposed and used in calculations of the evolution of quantum systems [16,17]. Efficient and stable simulation methods are needed to reduce the computation load and to increase the simulation speed.

The polynomial expansion method has been used in the calculation of dynamics and/or spectral properties of large quantum systems with great success [15,18–20], Tal-Ezer and Kosloff proposed an expansion in terms of Chebyshev polynomials and tested the method with the simple harmonic oscillator and the problem of scattering from a surface; very accurate results were obtained with an efficiency six times higher compared to the conventional scheme [15,19]. Silver and Röder used the Chebyshev polynomial expansion in the calculation of the density of states of a large sparse Hamiltonian matrix [20]. A fast evolution method based on the expansion of Chebyshev polynomial for dynamical quantum systems was proposed and checked by Loh *et al.* [21]. Dobrovitski *et al.* extended the Chebyshev polynomial expansion method in the study of a spin system interacting with a spin bath [9], obtained the decoherence properties of the system, and showed the efficiency and accuracy of the method. Since the Chebyshev polynomial is the most frequently used orthogonal polynomial in most numerical approximation theories [22], other kinds of orthogonal polynomials should also be applicable in the evolution problems. The argument of the Chebyshev polynomial is bounded to the interval $[-1,+1]$, which is suitable for systems with a bounded Hamiltonian, and for systems that are only bounded below, a cutoff for the energy spectrum is inevitable in order to use the method. However, it is well known that some of the orthogonal polynomials, like Hermite and Laguerre polynomials, do not limit their arguments to finite intervals. Expansion in terms of these kinds of orthogonal polynomials may have merit in unbounded systems. In this paper, we will explore the efficiency and accuracy of methods based on all these orthogonal polynomials. We constructed methods based on the Hermite and Laguerre polynomials and found that these orthogonal polynomials do have the required properties. The rest of the paper is organized as follows. In Sec. II, we briefly review the spin-bath model and the difficulty on getting its exact solution. In Sec. III, three kinds of polynomial scheme will be described for the expansion of the evolution operator. In Sec. IV, we present the results of our numerical simulation. Finally, a brief summary is given in Sec. V.

II. HAMILTONIAN

Two systems are used in this study to test the numerical methods. The first is a two-spin-1/2 system coupled to a spin environment and the second is a particle moving in a double-well potential.

The spin Hamiltonian we used in testing our numerical schemes is the one that was used in Refs. [9,23,24]. The system consists of two spins of 1/2 interacting antiferromagnetically, and the system is coupled to a bath of noninteracting spins 1/2. The Hamiltonian can be written as

$$H = 2J\mathbf{s}_1 \cdot \mathbf{s}_2 + \sum_k A_k(\mathbf{s}_1 + \mathbf{s}_2) \cdot \mathbf{I}_k. \tag{6}$$

Here $\mathbf{s}_1$ and $\mathbf{s}_2$ are two spins with spin 1/2 coupled by the coupling constant J, favoring the antiparallel alignment, which constitute the system. The spins $\mathbf{I}_k$, $k=1,2,\ldots,N$, are N spin-1/2 environment spins, interacting with the system by Heisenberg coupling A_k, and they do not interact with each other. The coupling constant between two system spins is much larger than the couplings to the environment spins, $J \gg A_k$. The couplings A_k are uniformly distributed in an interval. Both the system spins and the environment spins can be represented by Pauli matrices.

The Hilbert space of the whole system is 2^{N+2} dimensional when the environment consists of N spins. The basis state of the environment can be chosen as the direct product of the single states $|\uparrow\rangle$ or $|\downarrow\rangle$ for each spin $\vec{I}_k$; here $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of the square and z components of each spin. For a moderate size of the environment, say, $N=18$, we have to find an exact solution to about 10^6 differential equations. And when N is increased by 1, the number of equations is doubled. For this reason efficient algorithms are needed in studies of the evolution of this kind of problem, especially in the case of decoherence where a long simulation is required to reach the pointer state. Polynomial expansions based on both Chebyshev [9] and Hermite [25] polynomials are very successful in this case.

The Hamiltonian for the double-well potential is given by

$$H = \frac{p^2}{2} - \frac{1}{2}\omega^2 x^2 + \lambda x^4, \tag{7}$$

where we set $m=\hbar=1$. This model is very important in studies of critical phenomena and in the standard model of particle physics when the variable x is a scalar field. Here we take it to be a simple yet nontrivial model to test our numerical method.

III. POLYNOMIAL SCHEME

The formal solution of Eq. (4) is

$$\psi(t) = e^{-i\hat{H}t}\psi(0) = U(t)\psi(0). \tag{8}$$

The evolution operator $U(t)$ is an exponential functional of the Hamiltonian operator $\hat{H}$ which is represented as a matrix in the Hilbert space of ψ. The method of polynomial expansion is to expand the evolution operator $U(t)$ in terms of the orthogonal polynomials of Hamiltonian $\hat{H}$. The expansions in Chebyshev and Hermite polynomials are presented in [9,25], respectively. We will briefly introduce the Chebyshev and Hermite polynomial expansions and give a detailed derivation of expansion in terms of Laguerre polynomials, and check the efficiency of the method numerically.

A. Chebyshev polynomial

The Chebyshev expansion of $U(t)$ given by Dobrovitski *et al.* is

$$U(t) = \exp(-i\tau\tilde{H}) = \sum_{k=0}^{\infty} c_k T_k(\tilde{H}), \tag{9}$$

where $\tau = E_0 t/2$ and $\tilde{H} = 2\hat{H}/E_0$, E_0 is a scale factor, and T_k are the Chebyshev polynomials: $T_k(x) = \cos(k \arccos x)$. The reason that we change $\hat{H}$ into $\tilde{H}$ comes from the argument domain of $T_k(x)$, which is $x \in [-1, 1]$. For our spin system, $\hat{H}$ is bounded above and below, so that the scale factor E_0 can be determined in the following way:

$$E_{\max} = \max\langle\psi|\hat{H}|\psi\rangle,$$

$$E_{\min} = \min\langle\psi|\hat{H}|\psi\rangle,$$

$$E_0 = 2\ \max(|E_{\max}, E_{\min}|).$$

Using the orthogonal property of T_k, the expansion coefficients c_k of Eq. (9) can be calculated as

$$c_k = \frac{a_k}{\pi}\int_{-1}^{1} \frac{T_k \exp(-ix\tau)}{\sqrt{1-x^2}}\, dx = a_k(-i)^k J_k(\tau),$$

where $J_k(\tau)$ is the Bessel function of kth order, and $a_0 = 1$ when $k = 0$ and $a_k = 2$ when $k \geqslant 1$. The series of Chebyshev polynomials of Hamiltonian $\hat{H}$ can be calculated by the recursion process

$$T_0(\tilde{H}) = 1,$$

$$T_1(\tilde{H}) = \tilde{H},$$

$$T_{k+1}(\tilde{H}) = 2\tilde{H}T_k(\tilde{H}) - T_{k-1}(\tilde{H}).$$

B. Hermite polynomial

In order to obtain the expansion in terms of Hermite polynomials, we start from its generating function [26]

$$e^{-s^2+2sx} = \sum_{k=0}^{\infty} \frac{s^k}{k!} H_k(x), \tag{10}$$

where $H_k(x)$ denotes the Hermite polynomial of order k. The evolution operator (8) can be rearranged as

$$e^{-i\hat{H}t} = e^{-(t/2\lambda)^2} e^{-(-it/2\lambda)^2 + 2\lambda\hat{H}(-it/2\lambda)}. \tag{11}$$

The second part of the right-hand side of Eq. (11) is identified to be the generating function of the Hermite polynomial by setting $x = \lambda\hat{H}$ and $s = -it/2\lambda$ in Eq. (10), where λ is introduced for convenience. From Eqs. (10) and (11) we obtain the Hermite expansion form of the exponential operator $U(t)$:

$$e^{-i\hat{H}t} = e^{-(t/2\lambda)^2} \sum_{k=0}^{\infty} \frac{(-i)^k}{k!} (t/2\lambda)^k H_k(\lambda\hat{H}). \tag{12}$$

The formal solution $\psi(t) = \exp(-i\hat{H}t)\psi(0)$ then becomes

$$\psi(t) = e^{-(t/2\lambda)^2} \sum_{k=0}^{\infty} \frac{(-i)^k}{k!} (t/2\lambda)^k \phi_k,$$

$$\phi_k = H_k(\lambda\hat{H})\psi(0). \tag{13}$$

The Hermite polynomial of H can be obtained by the following recursive algorithm:

$$\phi_0 = \psi_0,$$

$$\phi_1 = 2\lambda\hat{H}\psi_0,$$

$$\phi_{k+1} = 2\lambda\hat{H}\phi_k - 2k\phi_{k-1}.$$

To discuss the convergence of the expansion, we consider the term when k is large. The Hermite polynomial may be replaced by its asymptotical expression [26]:

$$H_k(x) \approx 2^{(k+1)/2} k^{k/2} e^{-k/2 + x^2/2} \cos\left(\sqrt{2k+1}\,x - \frac{k\pi}{2}\right). \tag{14}$$

Substituting this into Eq. (12) and using Stirling's formula for the factorial,

$$k\,! \approx \exp[k(\ln k - 1)], \quad k \gg 1, \tag{15}$$

the magnitude of the kth term in the expansion of Eq. (12) for large k is

$$\frac{(t/2\lambda)^k}{k!} H_k(\lambda\hat{H}) \approx \frac{(t/\lambda)^k}{2^k e^{k(\ln k - 1)}} 2^{(k+1)/2} k^{k/2} e^{-k/2 + \lambda^2\hat{H}^2/2} \times \cos\left(\sqrt{2k+1}\,\lambda\hat{H} - \frac{k\pi}{2}\right). \tag{16}$$

The physically meaningful Hamiltonian should always be bounded below, and for every evolution problem, the spectrum of the system has a maximum value determined by the initial state, which is on the order of the total energy of the initial state. If we set a maximum energy E_m, a few times of the total energy, then the states with energy larger than this maximum will not enter the calculation, and we have a natural energy cut off of the problem, the E_m. Then we can replace $\hat{H}$ in Eq. (16) with E_m to estimate the condition of the convergence of the expansion:

$$\begin{aligned}
&\frac{(t/2\lambda)^k}{k!} H_k(\lambda E_m) \\
&\quad \leq 2^{-(k-1)/2} \exp\left[-\frac{k}{2}\ln k + \frac{k}{2} + \frac{\lambda^2 E_m^2}{2} + k\ln\left(\frac{t}{\lambda}\right)\right] \\
&\quad = 2^{-(k-1)/2} \exp\left\{-\frac{k}{2}\left[\ln k - \ln e + \ln\left(\frac{t}{\lambda}\right)^{-2} - \frac{\lambda^2 E_m^2}{k}\right]\right\} \\
&\quad = 2^{-(k-1)/2} \exp\left\{-\frac{k}{2}\left[\ln\left(\frac{k\lambda^2}{et^2}\right) - \frac{\lambda^2 E_m^2}{k}\right]\right\}.
\end{aligned}$$

From this expression we see that, if

$$\ln\left(\frac{k\lambda^2}{et^2}\right) - \frac{\lambda^2 E_m^2}{k} \geq 0,$$

or the time step t satisfies

$$t \leq \sqrt{\frac{k}{e}}\lambda \exp\left(-\frac{\lambda^2 E_m^2}{2k}\right), \tag{17}$$

and the kth term is not larger than $2^{-(k-1)/2}$, then the summation is convergent. In the numerical calculation given below, we set $\lambda=1/2$.

C. Laguerre polynomial

The expansion in terms of Laguerre polynomials can also be derived from its generating function [26]:

$$(1-s)^{-\alpha-1}e^{xs/(s-1)} = \sum_{k=0}^{\infty} L_k^{\alpha}(x)s^k \quad (|s|<1), \tag{18}$$

where α distinguishes different types of Laguerre polynomials. By setting $s=it/(\lambda+it)$ and $x=\lambda\hat{H}$, we get the Laguerre polynomial expansion as

$$\psi(t) = \left(\frac{\lambda}{\lambda+it}\right)^{\alpha+1}\sum_{k=0}^{\infty}\left(\frac{it}{\lambda+it}\right)^k \phi_k,$$

$$\phi_k = L_k^{\alpha}(\lambda\hat{H})\psi(0). \tag{19}$$

The recursion relation of Laguerre polynomials is

$$L_0^{\alpha}(x) = 1,$$

$$L_1^{\alpha}(x) = \alpha + 1 - x,$$

$$(k+1)L_{k+1}^{\alpha}(x) = (2k+\alpha+1-x)L_k^{\alpha}(x) - (k+\alpha)L_{k-1}^{\alpha}(x). \tag{20}$$

From this relation we obtain the Laguerre polynomial expansion of Hamiltonian $\hat{H}$ as

$$\phi_0^{\alpha} = \psi(0),$$

$$\phi_1^{\alpha} = (\alpha+1-\lambda\hat{H})\psi(0),$$

$$(k+1)\phi_{k+1}^{\alpha} = (2k+\alpha+1-\lambda\hat{H})\phi_k^{\alpha} - (k+\alpha)\phi_{k-1}^{\alpha}. \tag{21}$$

Different α's give different choices of the algorithm; the domain of α is in the interval of $(-1,\infty)$. In the calculation of the spin-bath Hamiltonian we use $\alpha=-1/2$ and set the parameter $\lambda=1$ for convenience. For other kinds of Hamiltonian different values of α may be used to attain higher efficiency and accuracy.

The convergence of the expansion of Eq. (19) is guaranteed by the relationship between Laguerre polynomial and Hermite polynomial [26]:

$$L_k^{-1/2}(x) = \frac{(-1)^k}{2^{2k}k!}H_{2k}(\sqrt{x}). \tag{22}$$

Substituting Eqs. (14), (15), and (22) into the expansion term $[it/(1+it)]^k L_k^{-1/2}(\hat{H})$ and replacing $\hat{H}$ with E_m, the total energy of the initial state, we could estimate its asymptotical absolute value by such a procedure:

$$\left|\left(\frac{it}{1+it}\right)^k L_k^{-1/2}(E_m)\right|$$

$$\approx \left(\frac{t^2}{\lambda^2+t^2}\right)^{k/2}\frac{1}{2^{2k}e^{k(\ln k-1)}}2^{(2k+1)/2}2^k k^k e^{-k+E_m/2}$$

$$\times\cos\left(\sqrt{2k+1}E_m - \frac{k\pi}{2}\right) \leq 2^{1/2}\left(\frac{t^2}{\lambda^2+t^2}\right)^{k/2} e^{E_m/2}$$

$$= \exp\left\{-k/2\left[\ln\left(\frac{1+t^2}{t^2}\right) - \frac{E_m+\ln 2}{k}\right]\right\}.$$

For large k and a suitably chosen time step

$$t < \left[\exp\left(\frac{E_m+\ln 2}{k}\right) - 1\right]^{-1/2}, \tag{23}$$

the terms approach zero exponentially.

It should be noted that the energy cutoff E_m is only used here for convergence proof. In practical calculations, we do not need to specify this cutoff and the time step is chosen by test and error.

Compared to the Chebyshev expansion, the methods of the Hermite and Laguerre polynomials have an obvious advantage that no scaling to the Hamiltonian is needed, so that these expansions may have wider applications. On the other hand, the recurrence relation for both Hermite and Laguerre polynomials is not numerically absolutely stable as compared to the recurrence relation of the Chebyshev polynomial, which is marginally stable [27]. This fact limits the number of terms in the expansion to some value $k_{\max}$; the effect of numerical instability has little effect for $k<k_{\max}$ and the effect starts to show up beyond this cutoff. In practical calculations $k_{\max}$ may be chosen to be 30, and the time step is set up accordingly with a specified error tolerance to get convergent results. The calculation schemes presented here are very general and are not dependent on the specific form of the Hamiltonian; however, the applicability should be tested for each kind of Hamiltonian before it can be used in practical simulations. The efficiencies of the three kinds of polynomial expansion are almost the same from our numerical calculation; careful comparison reveals that for the current models the Laguerre expansion with $\alpha=1/2$ is a little faster than the others.

IV. NUMERICAL SIMULATION

A. Test of the spin model

The efficiency of the Chebyshev expansion over the conventional method of calculation has already been determined by [9,23]. In this section we check numerically the efficiency of the three kinds of polynomial expansion by comparing the performance among the three expansions as well as with the predictor-corrector (PC) and Runge-Kutta (RK) methods for the spin-bath Hamiltonian given in Sec. II. We calculated two particular variables using the Hamiltonian: (i) the z-component oscillation of any one of the center spins, i.e., s_i^z, $i=1$ or 2, which demonstrates the decoherence rate of the system; (ii) the time dependence of von Neumann's entropy, i.e., $S_{vN}=-\mathrm{Tr}\rho\ln\rho$, which characterizes the entanglement

degree of the state of the system [5]. We use the same parameters as used in [9,23]: the exchange strength $J=16.0$ and A_k are uniformly distributed between 0 and 0.5. The initial condition of the system is $|\psi(0)\rangle=|\uparrow\downarrow\rangle$ or written as $|10\rangle$, and the environment is a normalized linear superposition of the product states of N spins with random coefficients. The time step is chosen as $\Delta t=0.036$, which is determined by a compromise between the convergence requirement $\mathrm{Tr}(\rho)=1$ and the speed of computation. All three schemes are implemented and tested; the results are consistent with those given by [9,23]. We also did the calculation with two widely used ordinary differential equation solvers, the predictor-corrector and Runge-Kutta methods. Because of the need for stability and speed, the time step in these two methods is almost 1/10 of that in the polynomial schemes. We found that the calculation costs of the three polynomial expansion schemes are very close to each other, with the Laguerre polynomial expansion slightly faster, and the results are practically the same. So we only give the data obtained by the Laguerre polynomial expansion in the following.

Figure 1 shows results for the oscillation of $s_1^z(t)$ and von Neumann's entropy $S_{vN}(t)$ of the spin-bath Hamiltonian with parameters given in the figure caption. The results are obtained by the Laguerre polynomial expansion method and are consistent with results by other methods we tested and those reported in the literature [9,23].

A comparison between computational costs of different methods with the same error tolerance is listed in Table I. From the table we see that (i) when N is very small, it is hard to distinguish the calculation speed of the two kinds of numerical computation method; (ii) in general, the speed of the polynomial scheme is about eight times as fast as that of the direct solution methods, i.e., the Runge-Kutta method (the corresponding data of the predictor-corrector method are almost the same as for RK); (iii) with increasing N, the speed advantage becomes more evident. All the data reported here are obtained on a microcomputer with Intel Pentium M Banias processor 1400 MHz, memory 256M.

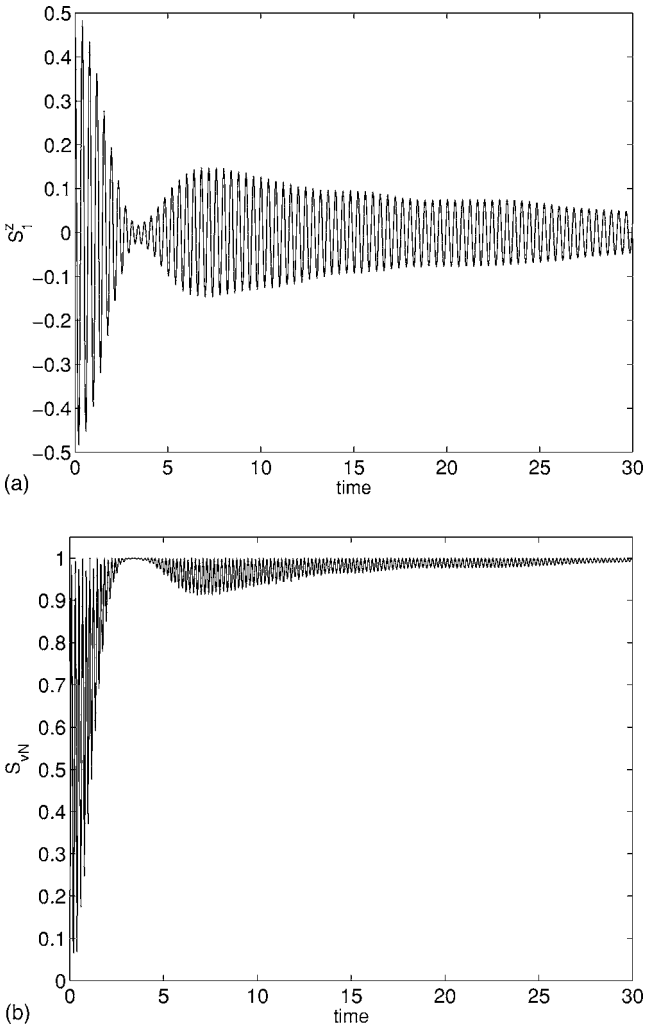

FIG. 1. Decoherence of two coupled spins by a spin bath calculated by the Laguerre method; the parameters are $J=16$, $N=12$; the tolerance in obtaining this figure is set to be 10^{-6}. (a) Oscillation of $s_1^z(t)$. (b) Evolution of entropy $S_{vN}(t)$.

B. The double-well model with Laguerre polynomial scheme

The Laguerre polynomial expansion scheme can easily be extended to the studies of continuous quantum systems. As an illustration, we used it in the calculation of the time evolution of a given wave function packet in a double-well system. The initial state was prepared as one of the eigenstates of a harmonic oscillator with unit mass and frequency ω, centered at the bottom of the right well, $x_0=\omega/\sqrt{4\lambda}$. That is,

$$\psi(0)=\left(\frac{\sqrt{\omega}}{\sqrt{\pi}2^m m!}\right)^{1/2} H_m[\sqrt{\omega}(x-x_0)]\exp[-\omega(x-x_0)^2/2]. \tag{24}$$

$H_m(x)$ is the Hermite polynomial of the mth order.

In order to use the Laguerre polynomial expansion scheme in the evaluation of the time evolution, we expand the state of the system to a complete basis state. In principle, any complete basis can be used in this calculation; however, a better choice of the basis will greatly reduce the computation efforts and obtain highly accurate results. In this study we use the eigenstates of a simple harmonic oscillator $\phi_n(x)$, $n=0,1,\ldots,\infty$, abbreviated as $|n\rangle$ as the expansion basis. The Hamiltonian of the simple harmonic oscillator that defines the basis is

TABLE I. Comparison of the RK method with the polynomial scheme (PS) for the problem of decoherence of a spin bath.

Scheme	Δt	No. of bath spins	Precision	t	CPU time (s)
RK	0.0036	4	10^{-6}	$9000\Delta t$	2
PS	0.036	4	10^{-6}	$900\Delta t$	2
RK	0.0036	8	10^{-6}	$9000\Delta t$	406
PS	0.036	8	10^{-6}	$900\Delta t$	50
RK	0.0036	10	10^{-6}	$9000\Delta t$	2065
PS	0.036	10	10^{-6}	$900\Delta t$	242

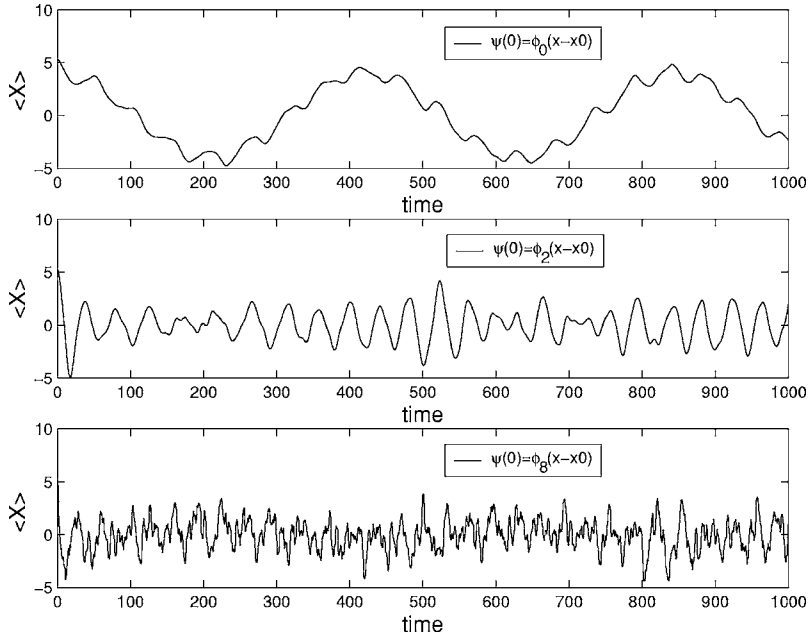

FIG. 2. The time evolution of $\langle x \rangle$ for three cases: (a) $\psi(0)=\phi_0(x-x_0)$; (b) $\psi(0)=\phi_2(x-x_0)$; (c) $\psi(0)=\phi_8(x-x_0)$. All of them are calculated for $\lambda/\omega=0.0013$.

$$h = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 x^2. \tag{25}$$

This is not necessarily the optimized basis; however, calculation shows that it is pretty good in this problem.

By introduction of the creation operator $a^\dagger$ and annihilation operator a, the matrix elements of the double-well Hamiltonian can easily be evaluated. The coordinate x and momentum p can be represented in terms of the operators $a^\dagger$ and a:

$$x = \sqrt{\frac{1}{2\omega}}(a^\dagger + a),$$

$$p = i\sqrt{\frac{\omega}{2}}(a^\dagger - a). \tag{26}$$

The actions of $a^\dagger$ and a on $|n\rangle$ are

$$a|n\rangle = \sqrt{n}|n-1\rangle, \tag{27}$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{28}$$

$$h|n\rangle = \omega\left(n + \frac{1}{2}\right)|n\rangle.$$

In the $a^\dagger$ and a representation, the double-well Hamiltonian (7) becomes

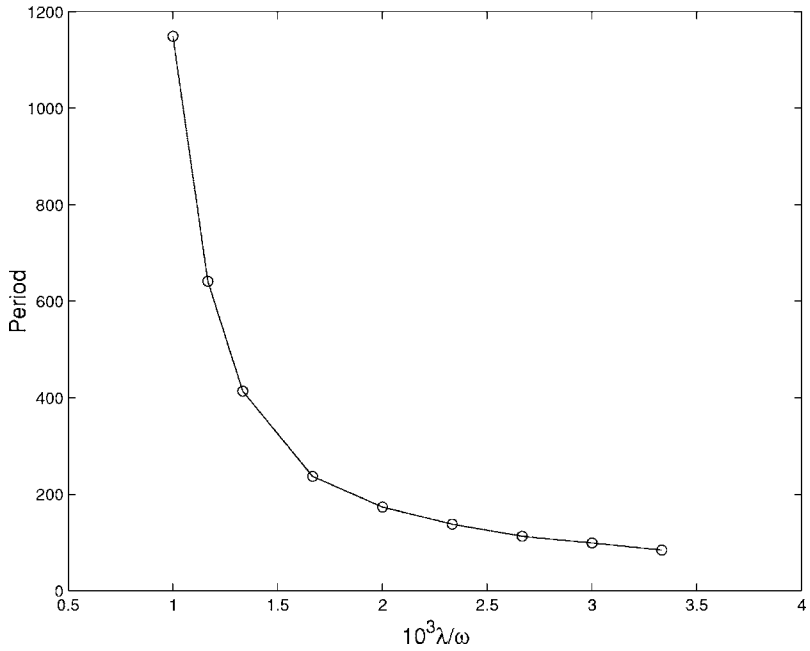

FIG. 3. Period of oscillation for different λ/ω with the same initial state $\psi(0)=\phi_0(x-x_0)$.

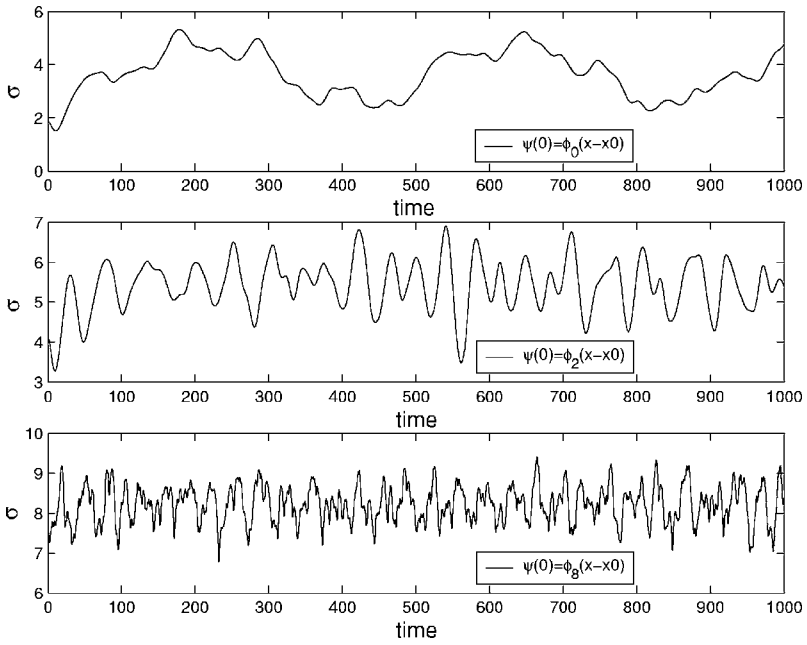

FIG. 4. Time evolution of standard deviation of coordinate $\sigma=(\langle x^2\rangle-\langle x\rangle^2)^{1/2}$ of three cases: $\psi(0)$= (a) $\phi_0(x-x_0)$; (b) $\phi_2(x-x_0)$; (c) $\phi_8(x-x_0)$. All of them are calculated for $\lambda/\omega=0.0013$.

$$H=-\frac{1}{2}\omega[(a^\dagger)^2+a^2]+\frac{\lambda}{4\omega^2}(a^\dagger+a)^4. \tag{29}$$

By using (27), the matrix elements of (29) can easily be obtained. The matrix form of the Hamitonian can be substituted directly in the Laguerre polynomial expansion scheme provided a suitable cutoff of the states is specified. In our calculation, we cut off the states at $n=49$, at which in all cases we studied the results are already convergent. The initial state $\psi(0)$ in the calculation is also expanded in terms of $|n\rangle$. When $m=0$ in (24), the expansion is

$$\psi(0)=\exp\left(-\frac{1}{2}\alpha_0^2\right)\sum_{n=0}^{N}\frac{\alpha_0^n}{\sqrt{n!}}|n\rangle,$$

$$\alpha_0=x_0\sqrt{\frac{\omega}{2}}.$$

For other values of m in (24), the coefficients of the expansion can easily be evaluated numerically.

Using the Laguerre polynomial scheme, we calculated the average position $\langle x\rangle$ and the variation $\sigma=(\langle x^2\rangle-\langle x\rangle^2)^{1/2}$. Figure 2 plots the evolution of the average position $\langle x\rangle$ with time. The initial states are the eigenstates of a simple harmonic centered at the right well of the double-well potential. For the state of $\phi_0(x-x_0)$, which is located at x_0 initially, it oscillates back and forth with time. From Fig. 2(a) we see clearly the periodic motion, and the period can easily be identified. The period depends on the value of λ/ω, smaller λ/ω corresponding to a deeper well and thus a longer period. Figure 3 plots the period as a function of the ratio λ/ω, which is decreasing monotonically as expected. For states of higher energies, though the initial state is also localized at the right potential well, the average position no longer follows a periodic oscillation between the two wells; instead, the particle spends most of the time moving around the center of the potential. Figure 4 shows plots of the variation of the position $\sigma=(\langle x^2\rangle-\langle x\rangle^2)^{1/2}$ as a function of time, which represents the width of the corresponding wave packet. From the figure, we see that for the low-energy state $\phi_0(x-x_0)$, the width is typically 4, as can be seen in the figure, smaller than the total width of the potential at the average energy of $\phi_0(x-x_0)$, which is about 10, and it looks like a wave packet bouncing about. The energy of the state $\phi_0(x-x_0)$ for the parameters chosen is −0.0390, slightly lower than the height of the middle peak of the potential. The movement of the center of the particle between the two wells is a case of quantum tunneling. In the higher-energy cases, the wave packet spends most of the time oscillating around the center of the potential well and there is no well defined period can be found.

A similar problem was studied by Bender *et al.* many years ago [28]. If we transform the x coordinate to q

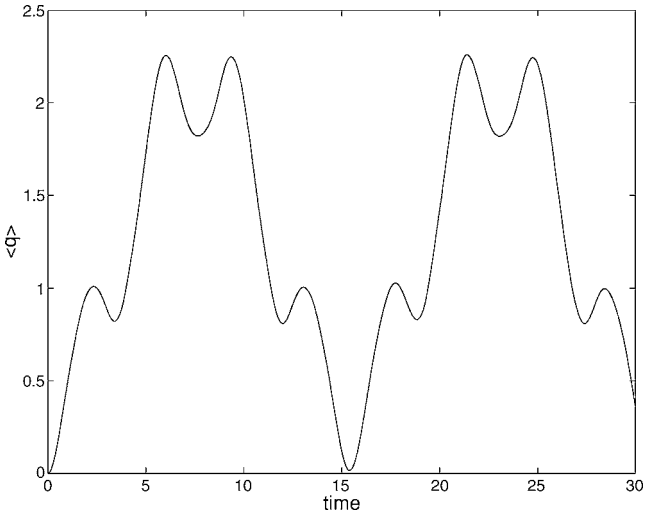

FIG. 5. Time dependence of $\langle q\rangle$ with $\beta=2.5$.

according to $q=x+\beta/2$ and set $\omega=\sqrt{8.0}$, Eq. (7) is changed into

$$H=\frac{1}{2}p^2+4q^2(q-\beta)^2/\beta^2, \tag{30}$$

which is exactly Eq. 1 in Ref. [28]. We use the same initial conditions as used in [28] to calculate $\langle q\rangle$ by our scheme (here the number of energy eigenstates N is truncated to 32, which is sufficient for convergence). The result is given in Fig. 5, which is the same as Fig. 1 in [28]. The calculation time for this figure is only about 4 s on a personal computer, Pentium(R) 4 CPU 2.60 GHz, memory 512M.

V. SUMMARY

In summary, we proposed a Laguerre polynomial expansion scheme, and tested its validity and efficiency by means of the spin-bath model and a continuous double-well model. The obvious merit of this scheme compared to the Chebyshev polynomial expansion scheme is that no scaling to the Hamiltonian is required, which means that *a priori* knowledge of the lower and upper bounds of the Hamiltonian is not needed. On the other hand, the computation efficiency and accuracy of the method are basically the same as for the Chebyshev polynomial expansion scheme.

We have also made use of the Laguerre expansion scheme in other kinds of model systems to study the effect of intrabath entanglement on the decoherence of the center spins. The method is also as efficient and accurate in those models as it was in the current spin-bath model. The results will be reported in separate presentations.

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